# Generative Adversarial Networks for Crystal Structure Prediction

Year: 2020 | Citations: 212 | Authors: Sungwon Kim, Juhwan Noh, Geun Ho Gu, A. Aspuru■Guzik, Yousung Jung

## Abstract

The constant demand for novel functional materials calls for efficient strategies to accelerate the materials discovery, and crystal structure prediction is one of the most fundamental tasks along that direction. In addressing this challenge, generative models can offer new opportunities since they allow for the continuous navigation of chemical space via latent spaces. In this work, we employ a crystal representation that is inversion-free based on unit cell and fractional atomic coordinates and build a generative adversarial network for crystal structures. The proposed model is applied to generate the Mg–Mn–O ternary materials with the theoretical evaluation of their photoanode properties for high-throughput virtual screening (HTVS). The proposed generative HTVS framework predicts 23 new crystal structures with reasonable calculated stability and band gap. These findings suggest that the generative model can be an effective way to explore hidden portions of the chemical space, an area that is usually unreachable when conventional substitution-based discovery is employed.